Project ID: mat153

A Multi-Scale Computational Platform for Predictive Modeling of Corrosion in Al-Steel Joints

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The University of Michigan

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Overview

Timeline

- Project start: **10/1/2018**
- Project end: **12/31/2021**
- Percent complete: **12%**

Budget

- Total project funding
  - DOE share: **$1,500,000**
  - Contractor share: **$478,431**

- Funding for FY2018 (expense)
  - DOE share: **$11,365**
  - Contractor share: **$3,589**

- Funding for FY2019 (budget)
  - DOE share: **$495,168**
  - Contractor share: **$154,456**

Barriers and Technical Targets

- Multi-material systems
- Aluminum – Steel joints
- Corrosion

- Develop predictive models for dissimilar Al-Steel joints (within 10% of experimental results) to enable mixed material structures

- 2017 U.S. DRIVE MTT Roadmap Report, Section 6

Partners

- Pennsylvania State University
- University of Illinois
- General Motors Company
- Optimal Process Technologies
- Livermore Software Technology Corp

Project lead: University of Michigan

Project Objective

- To develop and validate a model to predict the location and extent of corrosion in Al-steel joints and the impact of such corrosion on joint strength and fatigue life.

- The model will be validated by experiments with the goal of achieving strength and fatigue performance prediction accuracy within 10% of experimental results.

Relevance

- Prediction of the corrosion and its impact on performance of the dissimilar material joints is critical for reducing the massive number of the current corrosion-based recalls.
- Such models enable extensive use of the other multi-material systems for light-weighting.

Milestones

2019

Date	Milestone and Go/No Go Decisions	Status
March 2019	Milestone Material property survey	100%
June 2019	Milestone Fabrication of joints (RSW, SPR, R-W)	30%
Sept 2019	Milestone Thermodynamic DFT&CALPHAD models	On track
Dec 2019	Milestone Hybrid model for corrosion nucleation and growth	On track
Dec 2019	Go/No Go Decision Accelerated corrosion test that matches the form and degree of corrosion predicted by the models	On track

2020

Date	Milestone and Go/No Go Decisions	Status
March 2020	Milestone Joint characterization	On track
June 2020	Milestone Material property CALPHAD databases	On track
Sept 2020	Milestone Joint performance prediction	On track
Dec 2020	Milestone LS-DYNA platform model of material and joint performance	On track
Dec 2020	Go/No Go Decision Extended model of corrosion evolution	On track

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Predictive Modeling of Corrosion in Al-Steel Joints*

Approach / Strategy

1. Atomic-phase Level modeling with high throughput DFT and CALPHAD

2. Mesoscopic modeling with integrated uncertainty quantification

3. Macro-scale modeling for joint performance prediction

4. Dissimilar material joining and corrosion testing

5. Software integration

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Technical Accomplishments and Progress

✓ Defined the configuration of the joints and prepared coupons.

✓ Completed the set-up for joining using RSW and SPR.

✓ Planned the corrosion experimental tests at GM.

✓ Established the design of experiments for monitoring the corrosion evolution.

✓ Established the methods and the equipment to be used in quantification of the corrosion and mapping the location of the corrosion.
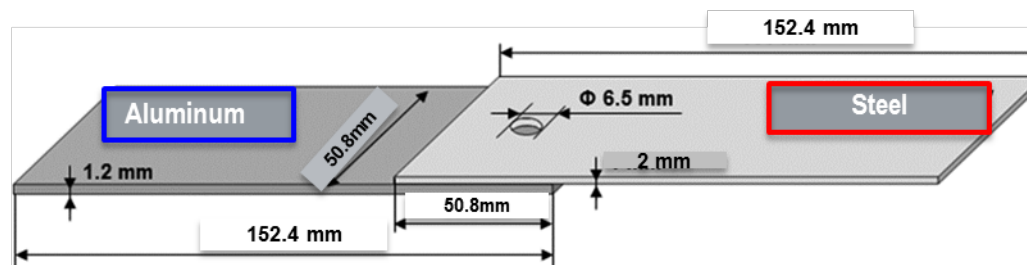

Materials: Aluminum: 1.2 mm AA 6022 and Steel: 2.0 mm HDG HSLA-340 (hot-dip galvanized steel)

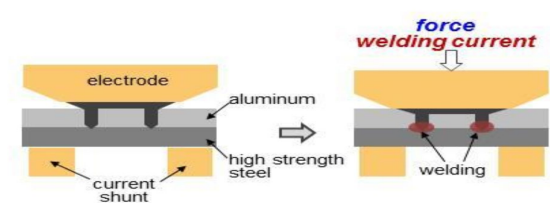# Technical Accomplishments and Progress
Joining processes

- ✓ Optimized the parameters for the SPR, RSW, and R-W to create samples of steel and aluminum alloy joints for subsequent examination, model development, and experiments.
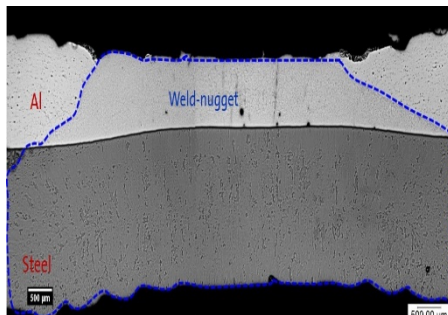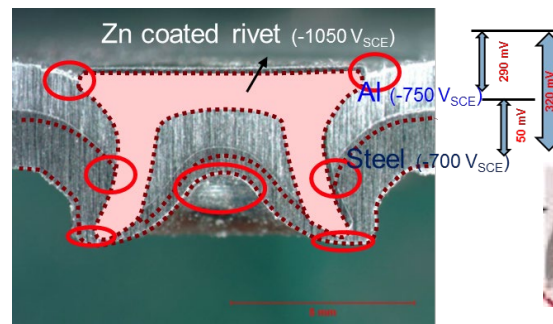- ✓ Analysed the critical areas where the corrosion is initiated.
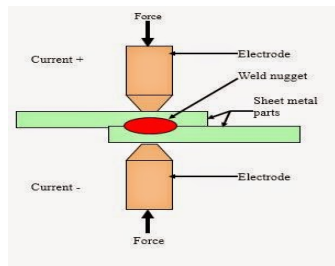
RSW
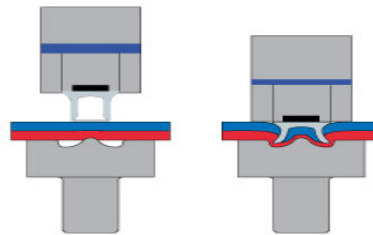
SPR

R-W

RSW Weld-nugget cross-section
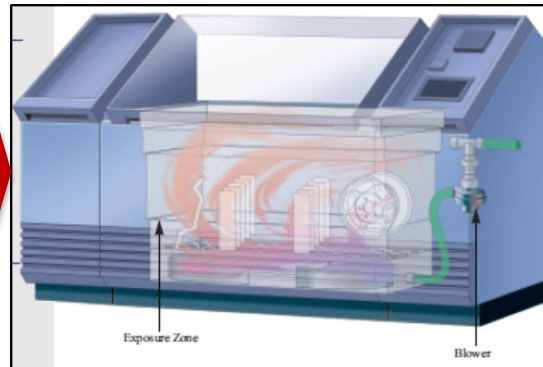[Courtesy of GM]

SPR cross-section
[Courtesy of GM]

Pullout failure of a R-W joint; cross section of joint
[Courtesy of Optimal]

Technical Accomplishments and Progress
Corrosion Experiments and Characterization

Field testing: desert, seashore, polluted city

Cabinet test

Custom cabinet test

Exposure conditions

– Environmental exposure chambers including a thermal cabinet and a cyclic corrosion cabinet (standards ASTM B117 and SAE J2334)

– Multi-channel potentiostat for DC and AC testing to salt fog

– Humidity chambers (ASTM D1748). The duration of the exposure will be between 1h~500h.

– A combination of all exposures can be programmed in cycles (typically a 24-hour cycle).

Duration of accelerated corrosion tests

– 50h, 200h, 300h, 400h, 1000h, 2000h [J. Hou, et al., 2016]

– 1 week, 2 week, 3 week, 4 week, 5 week, 6 week [W. T, et al., 2019]

– 1h, 5h, 25, 125h, 500h [C. Ma, et al., 2018]

– 20 days, 40 days, 60 days [H.L. Wan, et al., 2018]

– The maximum exposure time was set to 40 days

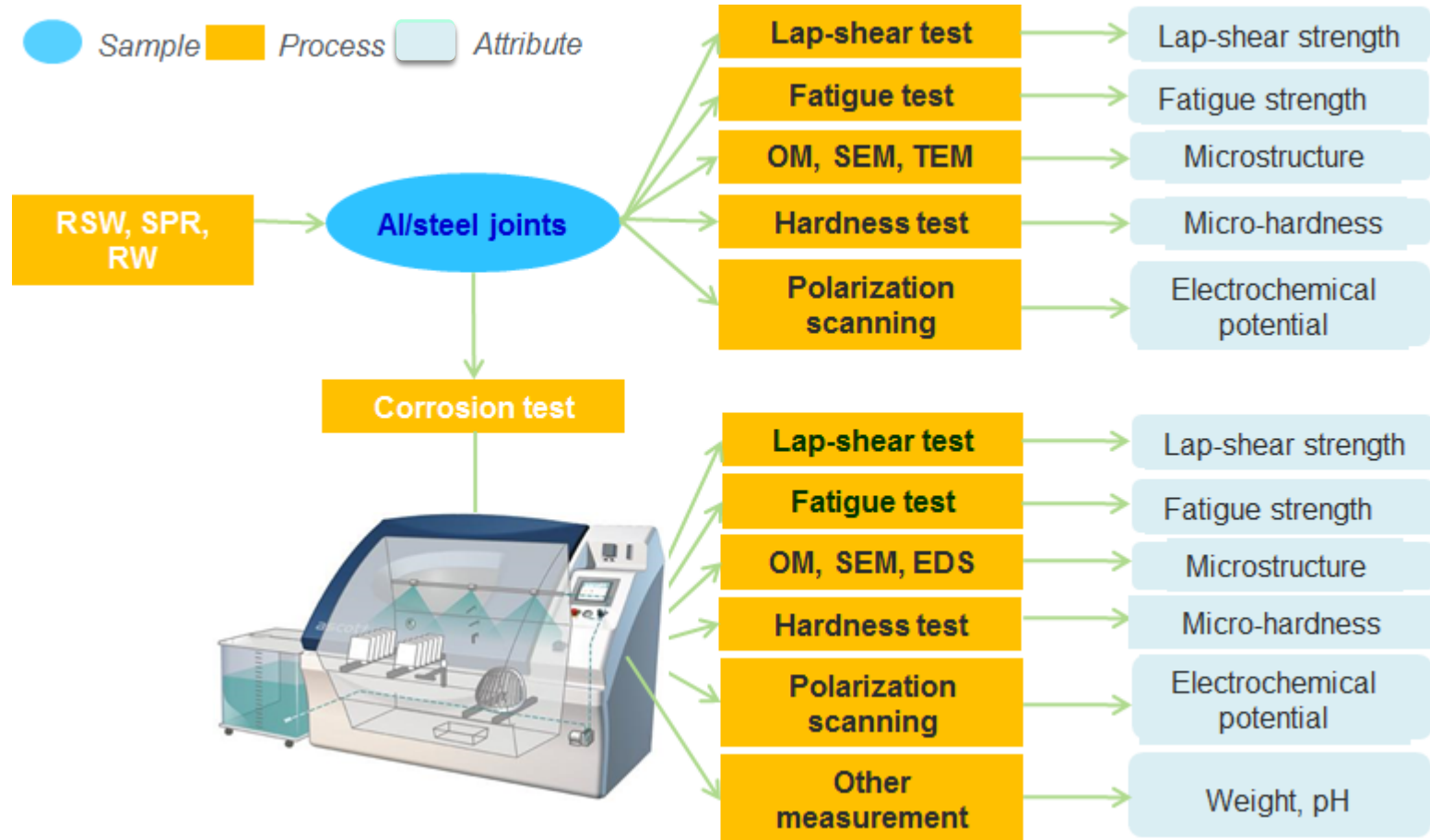– The maximum exposure time can be set between 500h to 1000h.

Technical Accomplishments and Progress

Preliminary corrosion tests done by GM
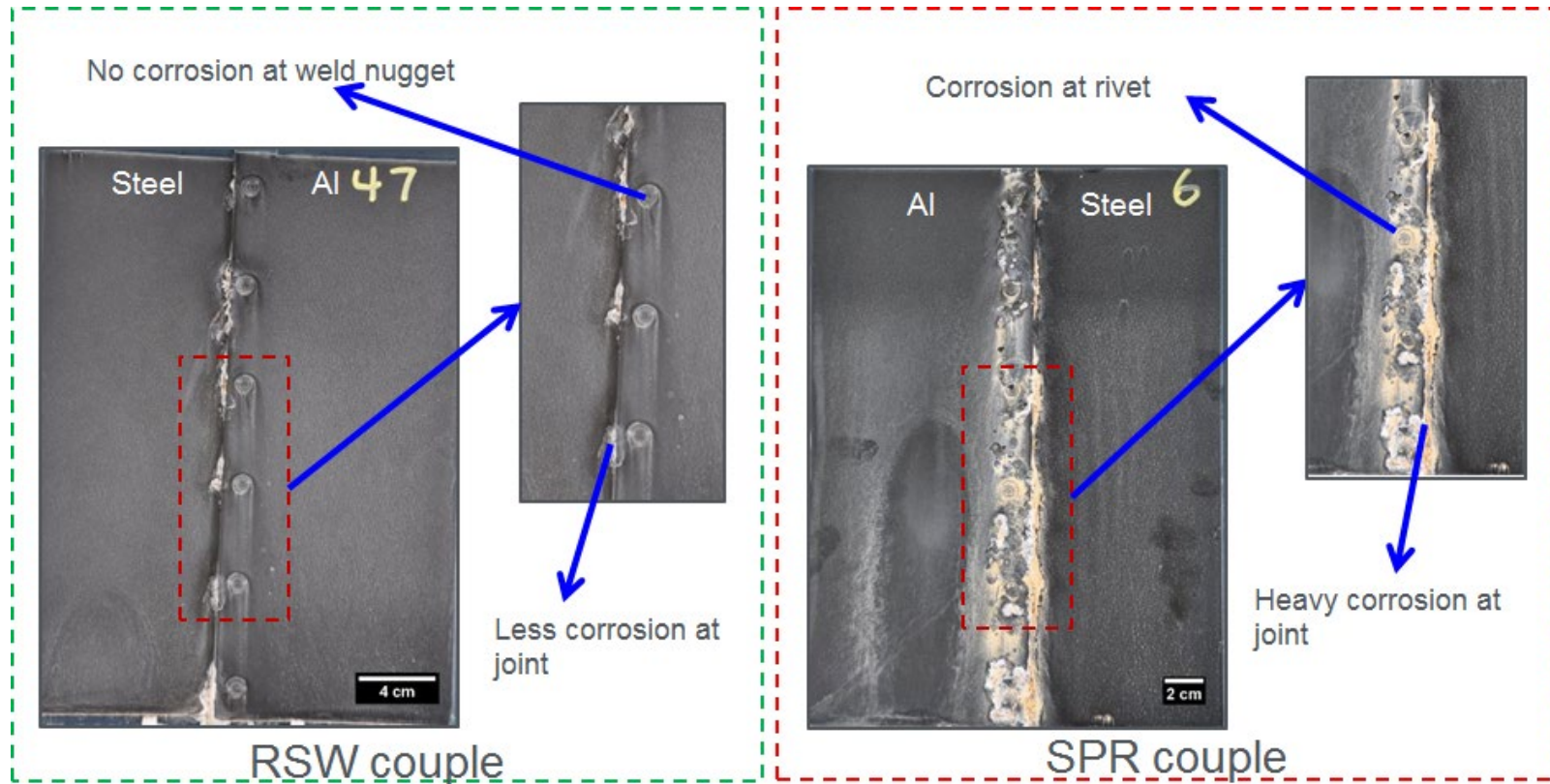
Technical Accomplishments and Progress
Workflow of the experimental characterization

Response to Previous Reviewers' Comments

This is a new start project and was
not previously reviewed.

Collaboration and Coordination with Other Institutions

University of Michigan – expertise in joining dissimilar materials and modeling the performance prediction.

Penn State University– expertise in joining of materials with a particular focus on mechanical behavior and interfacial phenomena, computational thermodynamics and kinetics and materials design.

University of Illinois– advanced statistics, machine learning, modeling uncertainty quantification, and high-performance computing (HPC). In this project, he will lead the tasks of developing methodologies for uncertainty quantification in multiscale modeling and building performance models for the SPR process.

Livermore Software Technology Corp - founded LSTC to commercialize as LS-DYNA the public domain code that originated as DYNA3D, originally developed at the Lawrence Livermore National Laboratory. LS-DYNA has been used in various industry, including Automobile Design, Aerospace, Manufacturing, and Bioengineering.

General Motors- provide facility for validation and demonstration of the technology based upon environmental exposure. Establish the standards for quantification of the corrosion in order to be able to accurately predict it.
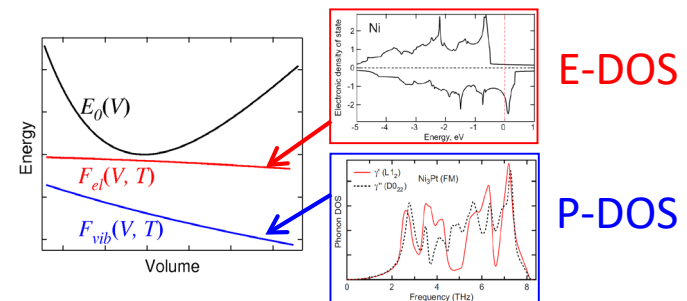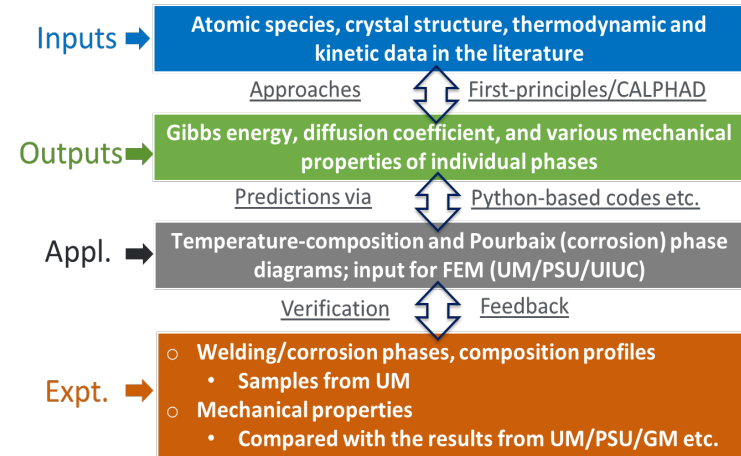
Optimal Process Technologies, LLC - provide innovative joining process technologies including the Rivet-Weld technology.
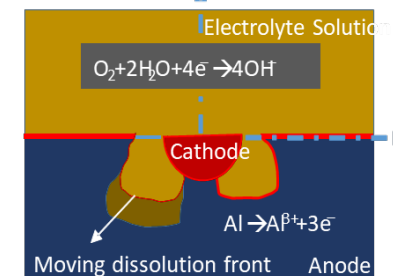
Remaining Challenges

- Prediction of corrosion initiation in RSW, SPR and R-W joints and experimental validation.

- The corrosion tests will be applied to E-coated joints to model the actual conditions of the joints in the car. Non-coated joints will corrode instantly leading to an impossibility of corrosion characterization.

- Consideration of the E-coat in the modeling is a challenge due to the complexity introduced by the e-coating film associated with the uncertainty of appearance new corrosion compounds.

- The team has considered this challenge and elaborated an approach to solve the problem.

Future Research

- **High Throughput CALPHAD Modeling and DFT Calculations**

- **DFT calculations of thermodynamic properties**

- **Finite Element based Mesoscopic Modeling of Corrosion Evolution**

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Any proposed future work is subject to change based on funding level.

Summary

- The configuration of the joints was set-up in agreement with General Motors. The aluminum and steel coupons were cut.

- Manufacturing of the RSW and SPR is in progress. OPT is in process of optimizing the parameters for R-W.

- The corrosion test set-up is prepared.

- The design of experiments for monitoring the corrosion evolution is done.

- The methods and the equipment to be used in quantification of the corrosion and mapping the location of the corrosion.

- The expected areas of corrosion for different joining process were identified based on the literature review and some preliminary results provided by GM.

- The intermetallic compounds of the interfaces created during joining were identified based on the theoretical analysis of the electrochemical potentials of the materials contributing to the joining.
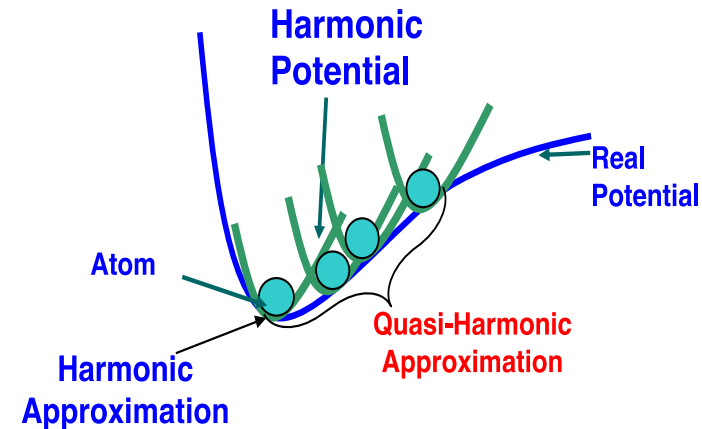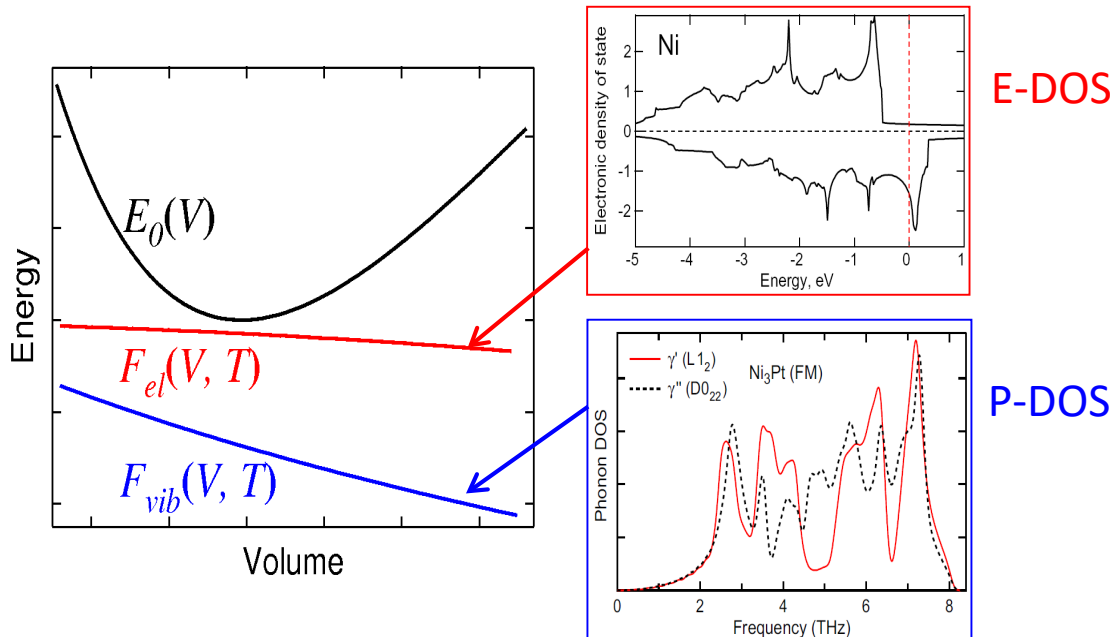
Back-up slides

Future Research
DFT calculations of thermodynamic properties

- **Quasi-Harmonic approach**

$$F(V,T) = E_0(V) + F_{vib}(V,T) + F_{el}(V,T)$$

- $E_0(V)$ — Static energy at 0 K and volume V, i.e., EOS (by VASP)
- $F_{vib}(V,T)$ — Vibrational contribution at V & T (Phonon or Debye model)
- $F_{el}(V,T)$ — Thermal electronic contribution at V & T (by VASP)

$E_0(V)$

$F_{el}(V, T)$

$F_{vib}(V, T)$

Energy

Volume

E-DOS

P-DOS

Harmonic Potential

Real Potential

Atom

Quasi-Harmonic Approximation

Harmonic Approximation

Acta Mater. 52 (2004), 2665, Comput. Mater. Sci. 47 (2010) 1040
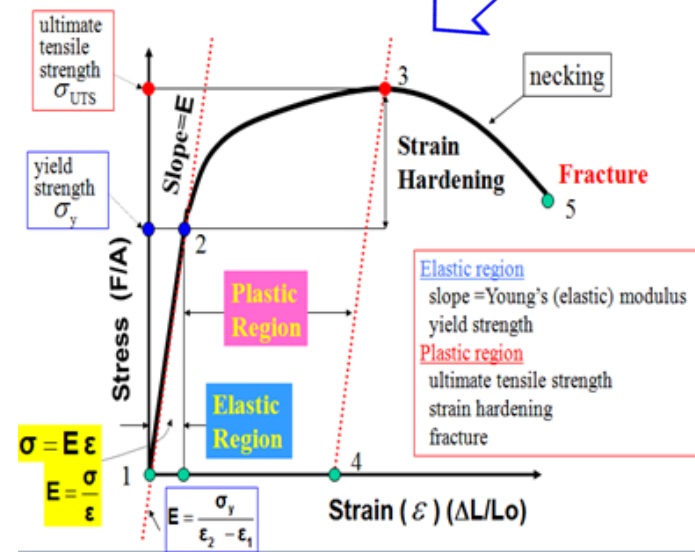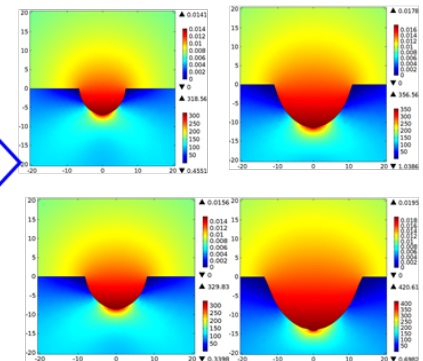
Future Research
Finite Element based Mesoscopic Modeling of Corrosion Evolution

- To simulate the evolution of corrosion from the modeling of electrochemical environment in crevices and pits due to galvanic corrosion in aqueous media, considering different conditions such as the coupling with the thermal & stress fields, the geometric parameters, and the electrode/electrolyte compositions and uncertainties.

- The developed mesoscopic corrosion models will serve as the application specific material behavior inputs for in-service joints performance predictions using continuum scale models to be developed in Task 4.

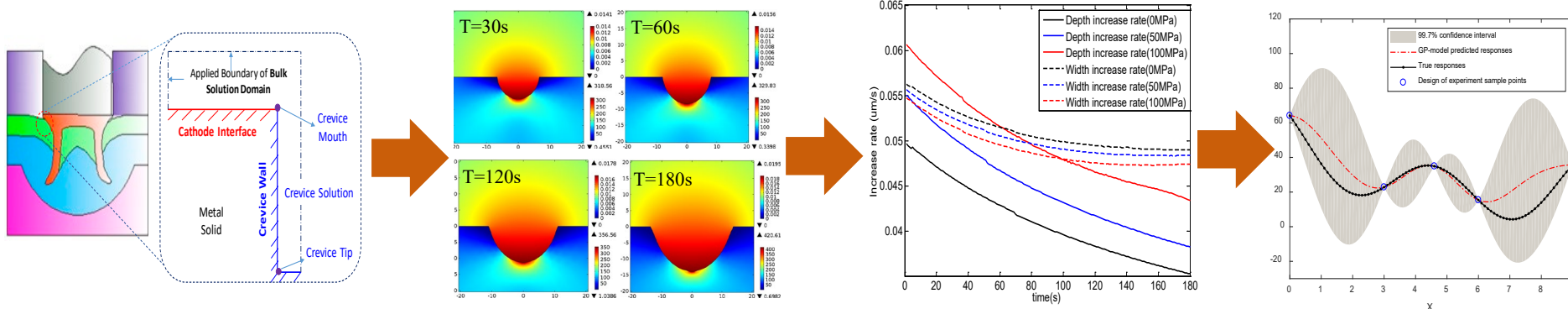*mat153: A Multi-Scale Computational Platform for Predictive Modeling of Corrosion in Al-Steel Joints*
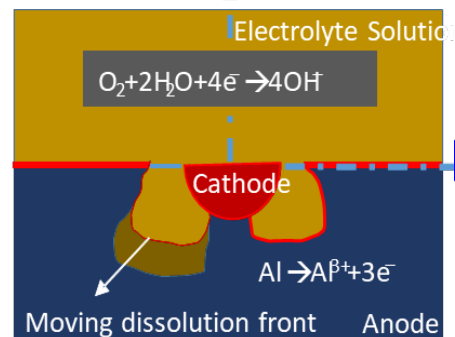
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Future Research
Finite Element based Mesoscopic Modeling of Corrosion Evolution
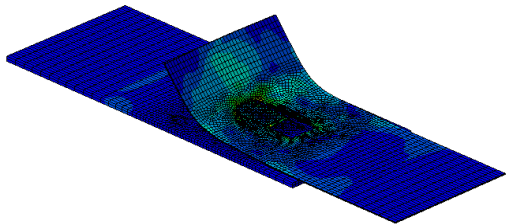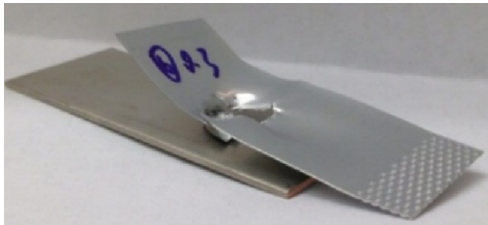
- **Task 3.1. Developing hybrid models for corrosion nucleation and growth**
  - Develop hybrid models that combine stochastic corrosion pit initiations and deterministic corrosion growth of established pit/crevice or a collection of pits.

- **Task 3.2. Corrosion Evolution Considering geometric and environmental factor couplings**
  - Extend the corrosion evolution models by considering the geometric and environmental factor couplings.

- **Task 3.3. Developing homogenized material models with uncertainty quantification**
  - UQ for the multi-scale corrosion simulation by integrating a novel probabilistic confidence-based adaptive sampling (PCAS) technique into the multi-scale simulation platform
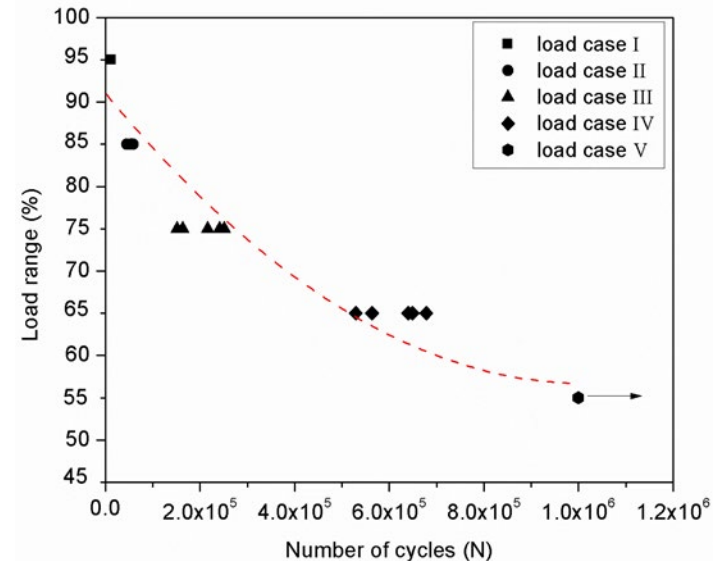

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Future Research
Joint Performance Modeling and Validation

4.1. Performance Prediction for Al-Steel Joints with Corrosion

4.2. Fatigue Life Models for RSW, SPR and R-W with Corrosion

4.3. Performance Prediction Models Validation

100 kN MTS Landmark Fatigue Test System

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Future Research
Software Integration &Technology Transfer

- The multi-scale models will be *integrated with existing commercial finite element software family, LS-DYNA,* for predicting the location and extent of corrosion and the impact of such corrosion on the performance of dissimilar materials joint.

- The multi-scale corrosion modeling platform based upon the LS-DYNA will be transferred to the industrial partners for validation and demonstration using practical industrial corrosion study data.

RSW   SPR   Rivet-Weld

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